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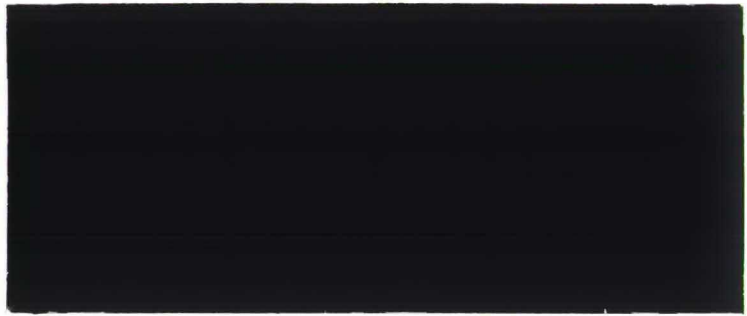
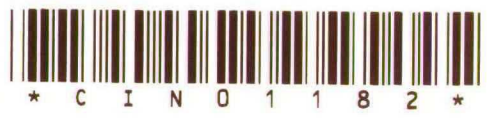
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**SENSITIVITY ANALYSIS OF SIMULATION  
EXPERIMENTS: REGRESSION ANALYSIS AND  
STATISTICAL DESIGN**

Jack P.C. Kleijnen

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SENSITIVITY ANALYSIS OF SIMULATION EXPERIMENTS:

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SENSITIVITY ANALYSIS OF SIMULATION EXPERIMENTS: REGRESSION ANALYSIS AND  
STATISTICAL DESIGN

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ABSTRACT

This tutorial gives a survey of strategic issues in the statistical design and analysis of experiments with deterministic and random simulation models. These issues concern what-if analysis, optimization, and so on. The analysis uses regression (meta)models and Least Squares. The design uses classical experimental designs such as  $2^{k-p}$  factorials, which are efficient and effective. If there are very many inputs, then special techniques such as group screening and sequential bifurcation are useful. Applications are discussed.

INTRODUCTION

Simulation is a mathematical technique that is applied in all scientific disciplines that use mathematical modeling, ranging from sociology to astronomy; also see Karplus [1]. It is a very popular technique because of its flexibility, simplicity, and realism. By definition, simulation involves experimentation, namely with the model of a real system. Consequently it requires on appropriate design and analysis. For real systems mathematical statistics has been applied since the 1930's: Sir Ronald Fisher focussed on agricultural experiments in the 1930's; George Box concentrated on chemical experimentation, since the 1950's; see [2]. Tom Naylor organized a conference on the design of simulation experiments back in 1968; see [3]. In 1974/75 my first book [4] covered both the 'tactical' and 'strategic' issues of experiments with random and deterministic

simulation models. The term tactical was introduced into simulation by Conway [5]; it refers to issues such as runlength and variance reduction, which arise only in random simulations such as queuing simulations. Strategic questions are: which combinations of input variables should be simulated, and how can the resulting output be analyzed? Obviously strategic issues arise in both random and deterministic simulations. Mathematical statistics can be applied to solve these questions, also in deterministic simulation; see the recent publications [6], [7], and [8]. This contribution focusses on these strategic issues in simulation experiments.

Strategic issues concern problems that are also addressed under names like model validation, what-if analysis, goal seeking, and optimization; see table 1, reproduced from my recent book [6, p. 136]. We shall return to this table.

#### REGRESSION METAMODELS

Before the systems analyst starts experimenting with the simulation model, he (or she) has accumulated prior knowledge about the system to be simulated: he may have observed the real system, tried different models, debugged the final simulation model, and so on. This tentative knowledge is formalized in a regression or Analysis of Variance (ANOVA) model. ANOVA models are elementary in the statistical theory of experimental design: Sums of Squares (SS's) are compared through the F test to detect significant main effects and interactions; see below. The simplest ANOVA models can be easily translated into regression models; see [6, pp. 263-293]. Because regression analysis is more familiar than ANOVA is, we shall use regression terminology henceforth.



Table 1: Terminology

Computer program	Simulation model	Regression model	User view
Output	Response	Dependent variable y	Result
Input	Parameter	Independent variable x	Environment
	Variable		
	Enumeration	Continuous	Validation Risk Analysis
	Function	Discrete	Controllable
	Scenario	Binary	Optimization
			Goal output (control)
			Satisfy (what-if)
	Behavioral relationship		

So prior knowledge is formalized in a tentative regression model. In other words, this model is tested later on to check its validity as we shall see. The regression model specifies which inputs seem important, which interactions among these inputs seem important, and which scaling seems appropriate. We shall discuss these items next.

Table 1 showed that 'inputs' are not only parameters and variables but may also be 'behavioral relationships'; that is, a module of the simulation model may be replaced by a different module. In the regression model such a qualitative change is represented by one or more binary (0,1) variables. Note that 'inputs' are called 'factors' in experimental design terminology. 'Interaction' means that the effect of a factor depends on the values (or 'levels') of another factor:

$$y = \beta_0 + \sum_{j=1}^k \beta_j x_j + \sum_{j=1}^k \sum_{g=1}^k \beta_{jg} x_j x_g + \sum_{j=1}^k \sum_{g=1}^k \sum_{h=1}^k \beta_{jgh} x_j x_g x_h + \dots + e, \quad (1)$$

where  $y$  is the simulation response;  $\beta_0$  is the overall or grand mean;  $\beta_j$  is the main or first-order effect of factor  $j$  ( $j = 1, \dots, k$ );  $\beta_{jg}$  is the two-factor interaction between the factors  $j$  and  $g$  ( $g = 1, \dots, k$ ;  $g \neq j$ );  $\beta_{jj}$  is the quadratic effect of factor  $j$ ;  $\beta_{jgh}$  is the three-factor interaction among the factors  $j$ ,  $g$ , and  $h$  ( $h = 1, \dots, k$ ;  $h \neq g \neq j$ ); and so on;  $e$  denotes 'fitting 'errors' or noise. Under certain strict mathematical conditions the 'response curve' in Eq. (1) is a Taylor series expansion of the simulation model  $y(x_1, \dots, x_k)$ . Unfortunately these conditions do not hold in simulation. Therefore we propose to start with an initial model that excludes interactions among three or more factors: such high-order interactions are popular in ANOVA but they are hard to interpret. The purpose of the regression model is to guide the design of the simulation experiment and to interpret the resulting simulation data; a regression model without high-order interactions suffices, as we observed repeatedly in practice.

The regression variables  $x$  in Eq. (1) may be transformations of the original simulation parameters and variables; for example,  $x_1 = \log(z_1)$  where  $z_1$  denotes the original simulation input. Scaling is also important: if the lowest value of  $z_1$  corresponds with  $x_1 = -1$  and its highest value corresponds with  $x_1 = +1$ , then  $\beta_1$  measures the relative importance of factor 1 when that factor ranges over the experimental area. In optimization we explore the response curve only locally if we use Response Surface Methodology (RSM). Then the local regression model is a first-order model:

$$y = \gamma_0 + \sum \gamma_j z_j + e, \quad (2)$$



where the importance of factor  $j$  at  $\bar{z}_j$ , the midpoint of the local experiment, is measured by  $r_j \bar{z}_j$ ; obviously  $\bar{z}_j = \sum_{i=1}^n z_{ij}/n = (L_j + H_j)/2$  where  $L_j \leq z_{ij} \leq H_j$  with local experimental area  $[L_1, H_1] \times \dots \times [L_k, H_k]$ ;  $z_{ij}$  denotes the value of factor  $j$  in simulation run or observation  $i$ . See [9] and [2].

In any experiment the analyst uses a model such as Eq. (1), explicitly or implicitly. For example, if he changes one factor at a time, then (implicitly) he assumes all interactions  $(\beta_{jg}, \beta_{jgh}, \dots)$  to be zero. Of course it is better to make the regression model explicit and to find a design that fits that model, as we shall see next. But first note that we call the regression model a metamodel because it models the input/output behavior of the underlying simulation model.

#### EXPERIMENTAL DESIGN

Based on a tentative regression (meta)model we select an experimental design. The design matrix  $D = (d_{ij})$  specifies the  $n$  combinations of the  $k$  factors that are to be simulated. (In multi-stage experimentation such as RSM that set of  $n$  combinations is followed by a next set.) Classical statistical theory gives designs that are 'efficient' and 'effective'. Efficiency means that the number of combinations or simulation runs is 'small'. Suppose there are  $Q$  effects in the regression model. The number of runs should satisfy the condition  $n \geq Q$ ; for example, we need  $k + 1$  runs if there are no interactions at all. So we may do one base run (say)  $x'_0 = (-1, -1, \dots, -1)$ ; and then we change one factor at a time:  $x'_1 = (+1, -1, \dots, -1)$ ,  $x'_2 = (-1, +1, -1, \dots, -1), \dots, x'_k = (-1, \dots, -1, +1)$ ; see table 2 for  $k = 3$ . However, to estimate the effects  $\underline{\beta}' = (\beta_0, \beta_1, \dots, \beta_k)$  we fit a curve to the simulation data  $(X, y)$  where  $X = (1, D)$  in the first-order model;  $1$  denotes a vector of  $n$  ones. The classical fitting criterion is Least Squares. This criterion yields the estimator

$$\hat{\underline{\beta}} = (X' X)^{-1} X' y. \quad (3)$$

Now consider the classical  $2^{3-1}$  design of Table 2. The corresponding  $X$  is orthogonal, so (3) reduces to the scalar expression

$$\hat{\beta}_{j'} = \sum_{i=1}^n x_{ij'} y_i / n \quad (j' = 0, 1, \dots, k). \quad (4)$$

Table 2. Two designs for three factors.

	One at a time			$2^{3-1}$ Design		
Run	d	d	d	d	d	d
	1	2	3	1	2	3
1	-	-	-	-	-	+
2	+	-	-	+	-	-
3	-	+	-	-	+	-
4	-	-	+	+	+	+

How can we choose between the two designs of table 2? Classical theory assumes that the fitting errors  $e$  are white noise:  $e$  is normally, and independently distributed with zero mean and constant variance (say)  $\sigma^2$ . Then (3) yields the variance-covariance matrix

$$\text{cov}(\hat{\beta}) = (X' X)^{-1} \sigma^2. \quad (5)$$

An orthogonal matrix  $X$  is optimal: it minimizes  $\text{var}(\hat{\beta}_j)$ , the elements on the main diagonal of Eq. (5); see [6, p.335]. There are straightforward procedures for deriving design matrices, if  $n = 2^{k-p}$  with  $(p=0,1,\dots)$ ; for other  $n$  values results are tabulated; see [2] and [6].

So the classical designs are efficient under the white noise assumption (recent research uses alternative assumptions; see Sachs et al. [7]). Moreover, these designs are effective: they permit the estimation of interactions. If we allow for two-factor interactions, then the number of

effects becomes  $Q = 1 + k + k(k-1)/2$ . If  $k$  is small, we may simulate  $n \geq Q$  combinations; for example, if  $k = 5$  then a  $2^{5-1}$  design is suitable. (If  $k$  is large, then we may hope that some factors will turn out to give nonsignificant main effects; we may assume that factors without main effects have no two-factor interactions either; there are designs that yield unbiased estimators for main effects with  $n = 2k < 1 + k + k(k-1)/2$ ; see [6, pp. 303 - 309], [9].) If the factors are quantitative, then a second-order regression model has  $k$  quadratic effects too. Then  $n$  must increase, and more than two levels per factor must be simulated: RSM designs; see [2] and [6].

### SCREENING

For didactic reasons we discuss 'screening' designs after classical experimental designs. In practice the simulation model has a great many factors that may be important; of course the analyst assumes that only a few factors are really important: parsimony. So in the beginning of a simulation study it is necessary to search for the few really important factors among the many conceivably important factors: screening.

Classical textbooks do not discuss screening situations, because in real-life experiments it is impossible to control (say) a hundred factors. In simulation, however, we perfectly control all inputs and we indeed use models with many inputs. One approach is group screening, introduced in the early 1960's by Watson, Jacoby and Harrison, Li, and Patel. This technique aggregates the many individual factors into a few group factors. Some simulation applications can be found in [6, p.327]. Recently Bettonvil [10] further developed group screening into sequential bifurcation, a very efficient technique that accounts for white noise and interactions. He applied this technique to an ecological model with nearly 300 factors.

## REGRESSION ANALYSIS: TECHNICALITIES

Eq. (3) gave the Ordinary Least Squares (OLS) estimator  $\hat{\beta}$ . In deterministic simulation that estimator may suffice, although Sachs et al. [7] give a better estimator if the white noise assumption is dropped (and replaced by a stationary covariance assumption). In random simulation the classical assumptions seldom hold. If the response variances differ with the inputs (as the response means do), then Weighted Least Squares (WLS) is better. If common random numbers drive the various factor combinations, then Generalized Least Squares (GLS) is best. See [6, pp. 161-175].

Once the regression model is calibrated (that is, the parameters  $\beta$  are estimated), the metamodel's validity must be tested. For deterministic simulation models we propose cross validation: delete factor combination  $i$  ( $x_i', y_i$ ); reestimate  $\hat{\beta}$  from the remaining simulation data ( $X_{-i}, y_{-i}$ ); predict the deleted response  $y_i$  through the reestimated regression model ( $\hat{y}_i = \hat{\beta}_{-i}' x_i$ ); "eyeball" the relative prediction errors  $\hat{y}_i/y_i$ : are these errors acceptable to the user?

In random simulation we prefer Rao's adjusted lack-of-fit F-test: the estimated response variances and covariances are compared with the residuals ( $\hat{y} - y$ ); see [11].

## SOME APPLICATIONS

Applications of our approach are getting numerous. For example, a simple - but realistic - case study concerns a Flexible Manufacturing System (FMS). Input to the FMS simulation is the 'machine mix', that is, the number of machines of type  $i$  with  $i = 1, \dots, 4$ . Intuitively selected combinations of these four inputs give inferior results when compared with a classical design. The throughput predicted by the simulation is analyzed through two different regression models. These models are validated. A regression model in only two inputs but including their interaction, gives valid predictions and sound explanations [12].

Another application concerns a decision support system (DSS) for production planning, developed for a Dutch company. To evaluate this DSS, a simulation model is built. The DSS has 15 control variables that are to



be optimized. The effects of these 15 variables are investigated, using a sequence of classical designs. Originally, 34 response variables were distinguished. These 34 variables, however, can be reduced to one criterion variable, namely productive machine hours, that is to be maximized, and one commercial variable measuring lead times, that must satisfy a certain side-condition. For this optimization problem the Steepest Ascent technique is applied to the experimental design outcomes. See [13].

A final case study concerns a set of deterministic ecological simulation models that require sensitivity analysis to support the Dutch government's decision making. First results for a model of the 'greenhouse' effect are given in [14]; additional results are given in [10].

#### CONCLUSIONS

Experimental design and regression analysis are statistical techniques that have been widely applied in the design and analysis of data obtained by real life experimentation and observation. In simulation, these techniques are gaining popularity: a number of case studies have been published. The techniques need certain adaptations to account for the peculiarities of deterministic and random simulations.

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## IN 1989 REEDS VERSCHENEN

- 368 Ed Nijssen, Will Reijnders  
"Macht als strategisch en tactisch marketinginstrument binnen de distributieketen"
- 369 Raymond Gradus  
Optimal dynamic taxation with respect to firms
- 370 Theo Nijman  
The optimal choice of controls and pre-experimental observations
- 371 Robert P. Gilles, Pieter H.M. Ruys  
Relational constraints in coalition formation
- 372 F.A. van der Duyn Schouten, S.G. Vanneste  
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- 373 Drs. R. Hamers, Drs. P. Verstappen  
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- 374 Rommert J. Casimir  
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- 375 Christian B. Mulder  
Efficient and inefficient institutional arrangements between governments and trade unions; an explanation of high unemployment, corporatism and union bashing
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On the estimation of a fixed effects model with selective non-response
- 377 J. Engwerda  
Admissible target paths in economic models
- 378 Jack P.C. Kleijnen and Nabil Adams  
Pseudorandom number generation on supercomputers
- 379 J.P.C. Blanc  
The power-series algorithm applied to the shortest-queue model
- 380 Prof. Dr. Robert Bannink  
Management's information needs and the definition of costs, with special regard to the cost of interest
- 381 Bert Bettonvil  
Sequential bifurcation: the design of a factor screening method
- 382 Bert Bettonvil  
Sequential bifurcation for observations with random errors

- 383 Harold Houba and Hans Kremers  
Correction of the material balance equation in dynamic input-output models
- 384 T.M. Doup, A.H. van den Elzen, A.J.J. Talman  
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- 385 Drs. R.T. Frambach, Prof. Dr. W.H.J. de Freytas  
Technologische ontwikkeling en marketing. Een oriënterende beschouwing
- 386 A.L.P.M. Hendrikx, R.M.J. Heuts, L.G. Hoving  
Comparison of automatic monitoring systems in automatic forecasting
- 387 Drs. J.G.L.M. Willems  
Enkele opmerkingen over het inversificerend gedrag van multinationale ondernemingen
- 388 Jack P.C. Kleijnen and Ben Annink  
Pseudorandom number generators revisited
- 389 Dr. G.W.J. Hendrikse  
Speltheorie en strategisch management
- 390 Dr. A.W.A. Boot en Dr. M.F.C.M. Wijn  
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Price adjustment in a two-country model
- 392 Martin F.C.M. Wijn, Emanuel J. Bijnen  
Prediction of failure in industry  
An analysis of income statements
- 393 Dr. S.C.W. Eijffinger and Drs. A.P.D. Gruijters  
On the short term objectives of daily intervention by the Deutsche Bundesbank and the Federal Reserve System in the U.S. Dollar - Deutsche Mark exchange market
- 394 Dr. S.C.W. Eijffinger and Drs. A.P.D. Gruijters  
On the effectiveness of daily interventions by the Deutsche Bundesbank and the Federal Reserve System in the U.S. Dollar - Deutsche Mark exchange market
- 395 A.E.M. Meijer and J.W.A. Vingerhoets  
Structural adjustment and diversification in mineral exporting developing countries
- 396 R. Gradus  
About Tobin's marginal and average  $q$   
A Note
- 397 Jacob C. Engwerda  
On the existence of a positive definite solution of the matrix equation  $X + A'X^{-1}A = I$

- 398 Paul C. van Batenburg and J. Kriens  
Bayesian discovery sampling: a simple model of Bayesian inference in auditing
- 399 Hans Kremers and Dolf Talman  
Solving the nonlinear complementarity problem
- 400 Raymond Gradus  
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- 402 Jack P.C. Kleijnen, Ben Annink  
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- 405 Harry Barkema  
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The use of the implied standard deviation as a predictor of future stock price variability: a review of empirical tests
- 411 Drs. J.C. Caanen en Dr. E.N. Kertzman  
Inflatieneutrale belastingheffing van ondernemingen
- 412 Prof. Dr. B.B. van der Genugten  
A weak law of large numbers for  $m$ -dependent random variables with unbounded  $m$
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A comparison of two lot sizing-sequencing heuristics for the process industry

- 414 C.B. Mulder en A.B.T.M. van Schaik  
Een nieuwe kijk op structuurwerkloosheid
- 415 Drs. Ch. Caanen  
De hefboomwerking en de vermogens- en voorraadaftrek
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- 417 Guido W. Imbens  
Efficient estimation of choice-based sample models with the method of moments
- 418 Harry H. Tigelaar  
On monotone linear operators on linear spaces of square matrices

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- 421 Steffen Jørgensen, Peter M. Kort  
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Regression Metamodels for Simulation with Common Random Numbers: Comparison of Techniques
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- 429 Theo van de Klundert en Anton B. van Schaik  
Liquidity Constraints and the Keynesian Corridor
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Central limit theorems for sequences with  $m(n)$ -dependent main part
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